

# Exploring the thermodynamic limit of Hamiltonian models: convergence to the Vlasov equation.

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We here discuss the emergence of Quasi Stationary States (QSS), a universal feature of systems with long-range interactions. With reference to the Hamiltonian Mean Field (HMF) model, numerical simulations are performed based on both the original  $N$ -body setting and the continuum Vlasov model which is supposed to hold in the thermodynamic limit. A detailed comparison unambiguously demonstrates that the Vlasov-wave system provides the correct framework to address the study of QSS. Further, analytical calculations based on Lynden-Bell's theory of violent relaxation are shown to result in accurate predictions. Finally, in specific regions of parameters space, Vlasov numerical solutions are shown to be affected by small scale fluctuations, a finding that points to the need for novel schemes able to account for particles correlations.

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The Vlasov equation constitutes a universal theoretical framework and plays a role of paramount importance in many branches of applied and fundamental physics. Structure formation in the universe is for instance a rich and fascinating problem of classical physics: The fossile radiation that permeates the cosmos is a relic of microfluctuation in the matter created by the Big Bang, and such a small perturbation is believed to have evolved via gravitational instability to the pronounced agglomerations that we see nowadays on the galaxy cluster scale. Within this scenario, gravity is hence the engine of growth and the Vlasov equation governs the dynamics of the non baryonic "dark matter" [1]. Furthermore, the continuous Vlasov description is the reference model for several space and laboratory plasma applications, including many interesting regimes, among which the interpretation of coherent electrostatic structures observed in plasmas far from thermodynamic equilibrium. The Vlasov equation is obtained as the mean-field limit of the  $N$ -body Liouville equation, assuming that each particle interacts with an average field generated by all plasma particles (i.e. the mean electromagnetic field determined by the Poisson or Maxwell equations where the charge and current densities are calculated from the particle distribution function) while inter-particle correlations are completely neglected.

Numerical simulations are presently one of the most powerful resource to address the study of the Vlasov equation. In the plasma context, the Lagrangian Particle-In-Cell approach is by far the most popular, while Eulerian Vlasov codes are particularly suited for analyzing specific model problems, due to the associated low noise level which is secured even in the non-linear

regime [2]. However, any numerical scheme designed to integrate the continuous Vlasov system involves a discretization over a finite mesh. This is indeed an unavoidable step which in turn affects numerical accuracy. A numerical (diffusive and dispersive) characteristic length is in fact introduced being at best comparable with the grid mesh size: as soon as the latter matches the typical length scale relative to the (dynamically generated) fluctuations a violation of the continuous Hamiltonian character of the equations occurs (see Refs. [3]). It is important to emphasize that even if such *non Vlasov* effects are strongly localized (in phase space), the induced large scale topological changes will eventually affect the system globally. Therefore, aiming at clarifying the problem of the validity of Vlasov numerical models, it is crucial to compare a continuous Vlasov, but numerically discretized, approach to a homologous  $N$ -body model.

Vlasov equation has been also invoked as a reference model in many interesting one dimensional problems, and recurrently applied to the study of wave-particles interacting systems. The Hamiltonian Mean Field (HMF) model [4], describing the coupled motion of  $N$  rotators, is in particular assimilated to a Vlasov dynamics in the thermodynamic limit on the basis of rigorous results [5]. The HMF model has been historically introduced as representing gravitational and charged sheet models and is quite extensively analyzed as a paradigmatic representative of the broader class of systems with long-range interactions [6]. A peculiar feature of the HMF model, shared also by other long-range interacting systems, is the presence of *Quasi Stationary States* (QSS). During time evolution, the system gets trapped in such states, which are characterized by non Gaussian velocity distributions, be-

fore relaxing to the final Boltzmann-Gibbs equilibrium [7]. An attempt has been made [8] to interpret the emergence of QSSs by invoking Tsallis statistics [9]. This approach has been later on criticized in [10], where QSSs were shown to correspond to stationary stable solutions of the Vlasov equation, for a particular choice of the initial condition. More recently, an approximate analytical theory, based on the Vlasov equation, which derives the QSSs of the HMF model using a maximum entropy principle, was developed in [11]. This theory is inspired by the pioneering work of Lynden-Bell [12] and relies on previous work on 2D turbulence by Chavanis [13]. However, the underlying Vlasov ansatz has not been directly examined and it is recently being debated [14].

In this Letter, we shall discuss numerical simulations of the continuous Vlasov model, the kinetic counterpart of the discrete HMF model. By comparing these results to both direct N-body simulations and analytical predictions, we shall reach the following conclusions: (i) the Vlasov formulation is indeed ruling the dynamics of the QSS; (ii) the proposed analytical treatment of the Vlasov equation is surprisingly accurate, despite the approximations involved in the derivation; (iii) Vlasov simulations are to be handled with extreme caution when exploring specific regions of the parameters space.

The HMF model is characterized by the following Hamiltonian

$$H = \frac{1}{2} \sum_{j=1}^N p_j^2 + \frac{1}{2N} \sum_{i,j=1}^N [1 - \cos(\theta_j - \theta_i)] \quad (1)$$

where  $\theta_j$  represents the orientation of the  $j$ -th rotor and  $p_j$  is its conjugate momentum. To monitor the evolution of the system, it is customary to introduce the magnetization, a macroscopic order parameter defined as  $M = |\mathbf{M}| = |\sum \mathbf{m}_i|/N$ , where  $\mathbf{m}_i = (\cos \theta_i, \sin \theta_i)$  stands for the microscopic magnetization vector. As previously reported [4], after an initial transient, the system gets trapped into Quasi-Stationary States (QSSs), i.e. non-equilibrium dynamical regimes whose lifetime diverges when increasing the number of particles  $N$ . Importantly, when performing the mean-field limit ( $N \rightarrow \infty$ ) *before* the infinite time limit, the system cannot relax towards Boltzmann-Gibbs equilibrium and remains permanently confined in the intermediate QSSs. As mentioned above, this phenomenology is widely observed for systems with long-range interactions, including galaxy dynamics [15], free electron lasers [16], 2D electron plasmas [17].

In the  $N \rightarrow \infty$  limit the discrete HMF dynamics reduces to the Vlasov equation

$$\partial f / \partial t + p \partial f / \partial \theta - (dV/d\theta) \partial f / \partial p = 0, \quad (2)$$

where  $f(\theta, p, t)$  is the microscopic one-particle distribu-

tion function and

$$V(\theta)[f] = 1 - M_x[f] \cos(\theta) - M_y[f] \sin(\theta), \quad (3)$$

$$M_x[f] = \int_{-\pi}^{\pi} \int_{-\infty}^{\infty} f(\theta, p, t) \cos \theta d\theta dp, \quad (4)$$

$$M_y[f] = \int_{-\pi}^{\pi} \int_{-\infty}^{\infty} f(\theta, p, t) \sin \theta d\theta dp. \quad (5)$$

The specific energy  $h[f] = \int \int (p^2/2) f(\theta, p, t) d\theta dp - (M_x^2 + M_y^2 - 1)/2$  and momentum  $P[f] = \int \int p f(\theta, p, t) d\theta dp$  functionals are conserved quantities. Homogeneous states are characterized by  $M = 0$ , while non-homogeneous states correspond to  $M \neq 0$ .

Rigorous mathematical results [5] demonstrate that, indeed, the Vlasov framework applies in the continuum description of mean-field type models. This observation corroborates the claim that any theoretical attempt to characterize the QSSs should resort to the above Vlasov based interpretative picture. Despite this, the QSS non-Gaussian velocity distributions have been *fitted* [8] using Tsallis'  $q$ -exponentials, and the Vlasov formalism assumed valid *only* for the limiting case of homogeneous initial conditions [14]. In a recent paper [11], the aforementioned velocity distribution functions were instead reproduced with an analytical expression derived from the Vlasov scenario, with no adjustable parameters and for a large class of initial conditions, including inhomogeneous ones. The key idea dates back to the seminal work by Lynden-Bell [12] (see also [18], [19]) and consists in coarse-graining the microscopic one-particle distribution function  $f(\theta, p, t)$  by introducing a local average in phase space. It is then possible to associate an entropy to the coarse-grained distribution  $\bar{f}$ : The corresponding statistical equilibrium is hence determined by maximizing such an entropy, while imposing the conservation of the Vlasov dynamical invariants, namely energy, momentum and norm of the distribution. We shall here limit our discussion to the case of an initial single particle distribution which takes only two distinct values:  $f_0 = 1/(4\Delta_\theta \Delta_p)$ , if the angles (velocities) lie within an interval centered around zero and of half-width  $\Delta_\theta$  ( $\Delta_p$ ), and zero otherwise. This choice corresponds to the so-called "water-bag" distribution which is fully specified by energy  $h[f] = e$ , momentum  $P[f] = \sigma$  and the initial magnetization  $\mathbf{M}_0 = (M_{x0}, M_{y0})$ . The maximum entropy calculation is then performed analytically [11] and results in the following form of the QSS distribution

$$\bar{f}(\theta, p) = f_0 \frac{e^{-\beta(p^2/2 - M_y[\bar{f}] \sin \theta - M_x[\bar{f}] \cos \theta) - \lambda p - \mu}}{1 + e^{-\beta(p^2/2 - M_y[\bar{f}] \sin \theta - M_x[\bar{f}] \cos \theta) - \lambda p - \mu}} \quad (6)$$

where  $\beta/f_0$ ,  $\lambda/f_0$  and  $\mu/f_0$  are rescaled Lagrange multipliers, respectively associated to the energy, momentum and normalization. Inserting expression (6) into the above constraints and recalling the definition of  $M_x[\bar{f}]$ ,  $M_y[\bar{f}]$ , one obtains an implicit system which can be

solved numerically to determine the Lagrange multipliers and the expected magnetization in the QSS. Note that the distribution (6) differs from the usual Boltzmann-Gibbs expression because of the “fermionic” denominator. Numerically computed velocity distributions have been compared in [11] to the above theoretical predictions (where no free parameter is used), obtaining an overall good agreement. However, the central part of the distributions is modulated by the presence of two symmetric bumps, which are the signature of a collective dynamical phenomenon [11]. The presence of these bumps is not explained by our theory. Such discrepancies have been recently claimed to be an indirect proof of the fact that the Vlasov model holds only approximately true. We shall here demonstrate that this claim is not correct and that the deviations between theory and numerical observation are uniquely due to the approximations built in the Lynden-Bell approach.

A detailed analysis of the Lynden-Bell equilibrium (6) in the parameter plane  $(M_0, e)$  enabled us to unravel a rich phenomenology, including out of equilibrium phase transitions between homogeneous ( $M_{QSS} = 0$ ) and non-homogeneous ( $M_{QSS} \neq 0$ ) QSS states. Second and first order transition lines are found that separate homogeneous and non homogeneous states and merge into a tricritical point approximately located in  $(M_0, e) = (0.2, 0.61)$ . When the transition is second order two extrema of the Lynden-Bell entropy are identified in the inhomogeneous phase: the solution  $M = 0$  corresponds to a saddle point, being therefore unstable; the global maximum is instead associated to  $M \neq 0$ , which represents the equilibrium predicted by the theory. This argument is important for what will be discussed in the following.

Let us now turn to direct simulations, with the aim of testing the above scenario, and focus first on the kinetic model (2)–(5). The algorithm solves the Vlasov equation in phase space and uses the so-called “splitting scheme”, a widely adopted strategy in numerical fluid dynamics. Such a scheme, pioneered by Cheng and Knorr [20], was first applied to the study of the Vlasov-Poisson equations in the electrostatic limit and then employed for a wide spectrum of problems [3]. For different values of the pair  $(M_0, e)$ , which sets the widths of the initial water-bag profile, we performed a direct integration of the Vlasov system (2)–(5). After a transient, magnetization is shown to eventually attain a constant value, which corresponds to the QSS value observed in the HMF, discrete, framework. The asymptotic magnetizations are hence recorded when varying the initial condition. Results (stars) are reported in figure 1(a) where  $M_{QSS}$  is plotted as function of  $e$ . A comparison is drawn with the predictions of our theory (solid line) and with the outcome of N-body simulation (squares) based on the Hamiltonian (1), finding an excellent agreement. This observation enables us to conclude that (i) the Vlasov equation governs the HMF

dynamics for  $N \rightarrow \infty$  both in the homogeneous and non homogeneous case; (ii) Lynden-Bell’s violent relaxation theory allows for reliable predictions, including the transition from magnetized to non-magnetized states.

Deviations from the theory are detected near the transition. This fact has a natural explanation and raises a number of fundamental questions related to the use of Vlasov simulations. As confirmed by the inspection of figure 1(b), close to the transition point, the entropy  $S$  of the Lynden-Bell coarse-grained distribution takes almost the same value when evaluated on the global maximum (solid line) or on the saddle point (dashed line). The entropy is hence substantially flat in this region, which in turn implies that there exists an extended basin of states accessible to the system. This interpretation is further validated by the inset of figure 1(a), where we show the probability distribution of  $M_{QSS}$  computed via N-body simulation. The bell-shaped profile presents a clear peak, approximately close to the value predicted by our theory. Quite remarkably, the system can converge to final magnetizations which are sensibly different from the expected value. Simulations based on the Vlasov code running at different resolutions (grid points) confirmed this scenario, highlighting a similar degree of variability. These findings point to the fact that in specific regions of the parameter space, Vlasov numerics needs to be carefully analyzed (see also Ref. [21]). Importantly, it is becoming nowadays crucial to step towards an “extended Vlasov theoretical model which enables to account for discreteness effects, by incorporating at least two particles correlations interaction term.

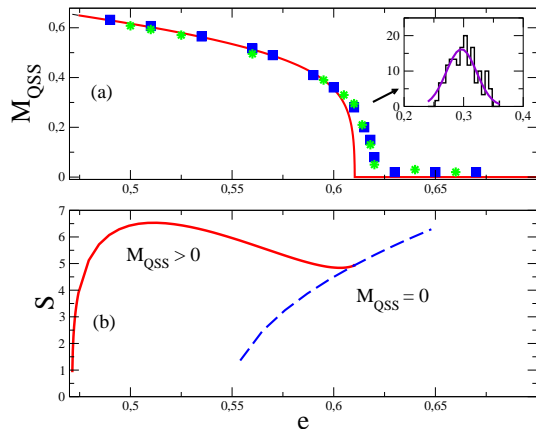


FIG. 1: Panel (a): The magnetization in the QSS is plotted as function of energy,  $e$ , at  $M_0 = 0.24$ . The solid line refers to the Lynden-Bell inspired theory. Stars (resp. squares) stand for Vlasov (resp. N-body) simulations. Inset: Probability distribution of  $M_{QSS}$  computed via N-body simulation (the solid line is a Gaussian fit). Panel (b): Entropy  $S$  at the stationary points, as function of energy,  $e$ : magnetized solution (solid line) and non-magnetized one (dashed line).

Qualitatively, one can track the evolution of the system in phase space, both for the homogeneous and non

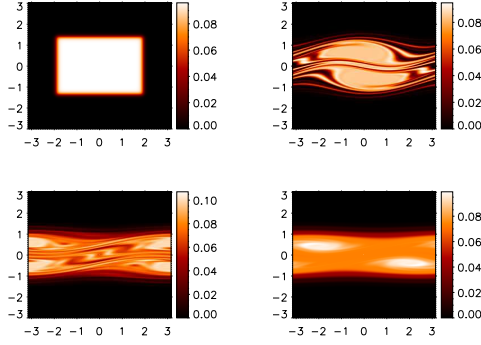


FIG. 2: Phase space snapshots for  $(M_0, e) = (0.5, 0.69)$ .

homogeneous cases. Results of the Vlasov integration are displayed in figure 2 for  $(M_0, e) = (0.5, 0.69)$ , where the system is shown to evolve towards a non magnetized QSS. The initial water-bag distribution splits into two large resonances, which persist asymptotically: the latter acquire constant opposite velocities which are maintained during the subsequent time evolution, in agreement with the findings of [11]. The two bumps are therefore an emergent property of the model, which is correctly reproduced by the Vlasov dynamics. For larger values of the initial magnetization ( $M_0 > 0.89$ ), while keeping  $e = 0.69$ , the system evolves towards an asymptotic magnetized state, in agreement with the theory. In this case several resonances are rapidly developed which eventually coalesce giving rise to complex patterns in phase space. More quantitatively, one can compare the velocity distributions resulting from, respectively, Vlasov and N-body simulations. The curves are displayed in figure 3 (a),(b),(c) for various choices of the initial conditions in the magnetized region. The agreement is excellent, thus reinforcing our former conclusion about the validity of the Vlasov model. Finally, let us stress that, when  $e = 0.69$ , the two solutions (resp. magnetized and non magnetized) [11] are associated to a practically indistinguishable entropy level (see figure 3 (d)). As previously discussed, the system explores an almost flat entropy landscape and can be therefore be stuck in local traps, because of finite size effects. A pronounced variability of the measured  $M_{QSS}$  is therefore to be expected.

In this Letter, we have analyzed the emergence of QSS, a universal feature that occurs in systems with long-range interactions, for the specific case of the HMF model. By comparing numerical simulations and analytical predictions, we have been able to unambiguously demonstrate that the Vlasov model provides an accurate framework to address the study of the QSS. Working within the Vlasov context one can develop a fully predictive theoretical approach, which is completely justified from first principles. Finally, and most important, results of conventional Vlasov codes are to be critically scrutinized,

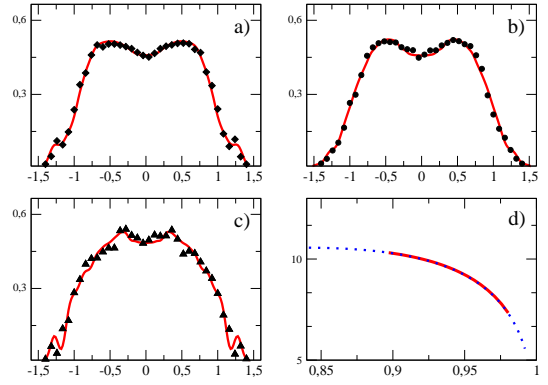


FIG. 3: Symbols: velocity distributions computed via N-body simulations. Solid line: velocity distributions obtained through a direct integration of the Vlasov equation. Here  $e = 0.69$  and  $M_0 = 0.3$  (a),  $M_0 = 0.5$  (b),  $M_0 = 0.7$  (c). Panel (d): Entropy at the stationary points as a function of the initial magnetization: the solid line refers to the global maximum, while the dotted line to the saddle point.

especially in specific regions of parameters space close to transitions from homogeneous to non homogeneous states.

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